

Thermal rectification in asymmetric U-shaped graphene flakes

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In this paper, we study the thermal rectification in asymmetric U-shaped graphene flakes by using nonequilibrium molecular dynamics simulations. The graphene flakes are composed by a beam and two arms. It is found that the heat flux runs preferentially from the wide arm to the narrow arm which indicates a strong rectification effect. The dependence of the rectification ratio upon the heat flux, the length and the width of the beam, the length and width of the two arms are studied. The result suggests a possible route to manage heat dissipation in U-shaped graphene based nanoelectronic devices.

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Graphene, a single layer of carbon atoms arranged in a honeycomb lattice, has attracted much interest due to its extraordinary properties[1, 2]. Since graphene exhibits much greater electron mobility than silicon as a zero band gap semiconductor, it has been considered as a promising candidate for the post-CMOS (complementary metal-oxide-semiconductor) material to replace silicon which is approaching its fundamental limit[3]. As electronic devices would undergo dramatic miniaturization, thus heat dissipation has become one of the most important barriers of breaking through. To achieve better functionality and longer lifetime for nanoelectronic devices, it is desirable to have in-depth understanding of the thermal properties of graphene which stimulates intense efforts both experimentally[4–6] and theoretically[7, 8]. To design a nanoelectronic device with better heat dissipation capacity, one of the most challenging issues is to design thermal rectifiers. Thermal rectification is a phenomenon that the heat flux runs preferentially in one direction and inferiorly in the opposite direction[9, 10]. Thus realization thermal rectification in graphene has deep implication for graphene based devices. Through molecular dynamics simulations, researchers have proposed several different thermal rectifiers from the asymmetric graphene nanoribbons[11–14]. In nanoelectronic designs, U-shaped devices are very common and widely used as electronic transistors and logic gates. Very recently it is found that the U-shaped graphene flakes reveal extremely high I_{on}/I_{off} ratio as channel transistors in experiments and they can easily realize and control the resonant tunneling without any external gates[15, 16]. The U-shaped graphene flakes can be fabricated by using lithography or gallium focused ion beam to cut from continuous graphene sheets[15, 16]. Therefore it arouses great interest to design thermal rectifiers by U-shaped graphene flakes.

Here we study the thermal rectification in asymmetric U-shaped graphene flakes by NEMD (nonequilibrium molecular dynamics) simulations. The graphene flakes are composed by a beam and two arms. We report that higher thermal conductivity is obtained when the heat flux runs from the wide arm to the narrow arm. We also discuss the impacts of the heat flux, the length and the width of the beam, the length and width of the two arms on the rectification ratio. Our result may inspire the experimentalists to realize thermal rectification in

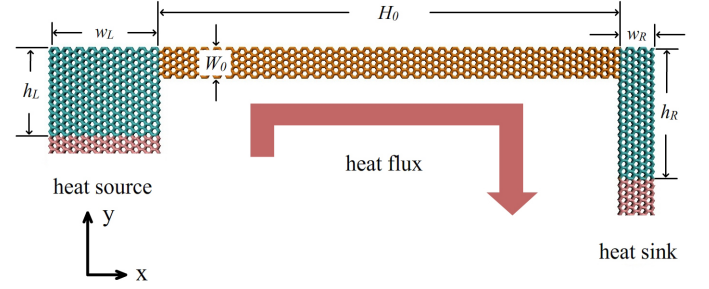


Figure 1: (Color online) Schematic of the U-shaped graphene flakes. The graphene flakes are composed by a beam and two arms. The heat source and heat sink are connected to the two arms. The heat flux runs from the heat source to the heat sink.

U-shaped graphene flakes.

In Fig. 1 we show the structure of the U-shaped graphene flakes. The graphene flakes are composed by a beam and two arms. The beam is drawn in orange with a length of H_0 and a width of W_0 . Different H_0 and W_0 are applied to investigate the dependence of thermal rectification ratio upon the size of the beam. The left arm is drawn in cyan with a length of h_L and a width of w_L . The right arm is also drawn in cyan with a length of h_R and a width of w_R . Different ratio of h_R/h_L and w_R/w_L are applied to investigate the dependence of thermal rectification upon the structural asymmetry. The end of the two arms is connected with either the heat source or the heat sink. The heat source and heat sink are drawn in red. Their outmost edges are frozen which is corresponding to fixed boundary condition. The heat flux runs from the heat source to the heat sink. We use the same reactive empirical bond-order (REBO) potential[17] as implemented in the LAMMPS[18] code to simulate the anharmonic coupling between the carbon atoms. Equations of motions are integrated with velocity Verlet algorithm with the minimum timestep $\Delta t = 0.25$ fs.

First the graphene flakes are equilibrated at a constant temperature $T = 300$ K in the Nose-Hoover thermostat by 0.75 ns. After that the heat flux is imposed. It is realized by the energy and momentum conserving velocity rescaling algorithm developed by Jude and Jullien[19]. It is widely used to investigate thermal rectification in different materials[20, 21].

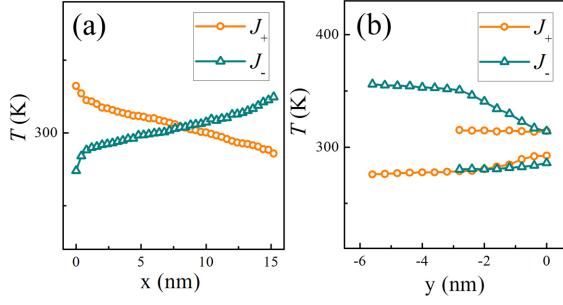


Figure 2: (Color online) (a) Typical temperature profiles on the beam. (b) Typical temperature profiles on the two arms. The left arm is shorter than the right arm.

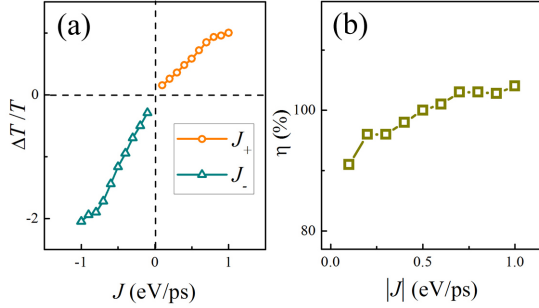


Figure 3: (Color online) (a) Heat flux J vs temperature differences $\Delta T/T$ between the two arms. J_+ corresponds to $\Delta T_+ > 0$ and J_- corresponds to $\Delta T_- < 0$. (b) Thermal rectification ratio η vs heat flux J .

By rescaling atomic velocities at each time step dt , specific amount of kinetic energy dE is added in the heat source and removed in the heat sink respectively. The heat flux can be calculated by $J = dE/dt$. The temperature profiles of the beam and the two arms are obtained by dividing the graphene flakes by several slabs of a constant length 4 \AA along their axis respectively. The local temperature of each slab is derived from the averaged kinetic energy. We average the temperature profiles over 100 ps after the heat flux is imposed. After 2 ns the temperature profiles do not change much and the whole nonequilibrium simulation process covers 3 ns.

The heat flux runs from the heat source to the heat sink along the U-shaped graphene flakes. We label the heat flux as J_+ ($J_+ > 0$) when the heat source is connected to the left arm and the heat sink is connected to the right arm. Similarly we label the reversed heat flux as J_- ($J_- < 0$) when the heat source is connected to the right arm and the heat sink is connected to the left arm. Due to the thermal rectification effect, different temperature profiles would be obtained by reversing the heat flux. According the Fourier's Law, thermal conductivity of the U-shaped graphene flakes can be qualified as:

$$G_+ = \frac{J_+/A}{\Delta T_+/L} \quad G_- = \frac{J_-/A}{\Delta T_-/L} \quad (1)$$

Here A is the averaged cross section, L is the distance between

the two arms, ΔT_+ (ΔT_-) is the temperature difference between the left arm and the right arm when J_+ (J_-) is imposed. Since $J_+ = -J_-$, A and L are the same, so the thermal rectification ratio η is qualified as[9, 20–22]:

$$\eta = \frac{G_+ - G_-}{G_-} = \left(\frac{-\Delta T_-}{\Delta T_+} - 1 \right) \times 100\% \quad (2)$$

In Fig. 2 we show the typical temperature profiles on the beam and the two arms. Here $J_{\pm} = \pm 0.1 \text{ eV/ps}$, $H_0 = 156.6 \text{ \AA}$, $W_0 = 9.7 \text{ \AA}$, $h_L = 27.9 \text{ \AA}$, $w_L = 36.4 \text{ \AA}$, $h_R = 54.6 \text{ \AA}$, $w_R = 4.0 \text{ \AA}$. The axis of the beam is in the x-axis while the axes of the two arms are in the y-axis. As shown in Fig. 2(a), there is no obvious difference between the two temperature profiles on the beam by imposing the heat flux J_+ and J_- respectively. Meanwhile, as shown in Fig. 2(b), distinctively different temperature drops between the two arms are observed by imposing the heat flux J_+ and J_- respectively. The temperature drop is much smaller by imposing the heat flux J_+ , therefore it indicates that the preferential direction is from the left arm (the wide arm) to the right arm (the narrow arm). The result also implies that the thermal rectification effect is caused by the asymmetric arms rather than the beam.

In order to illustrate the dependence of rectification ratio upon the heat flux, different heat fluxes are applied. In Fig. 3(a) we show the heat flux J_{\pm} versus the temperature difference $\Delta T_{\pm}/T$ between the two arms. It shows that the decreasing of the temperature difference under J_- is more steeply than the corresponding increasing of the temperature difference under J_+ . The result indicates again that the U-shaped graphene flake behaves like good thermal conductor under J_+ and poor thermal conductor under J_- . The heat flux runs preferentially from the wide arm to the narrow arm. It is similar to the rectification effect observed in asymmetric graphene nanoribbons where the preferred direction is along the direction of the decreasing width[11, 12]. In Fig. 3(b) we show the quantitative dependence of thermal rectification ratio upon the heat flux. With $J_{\pm} = \pm 0.1 \text{ eV/ps}$ the rectification ratio is 91%, while with $J_{\pm} = \pm 1.0 \text{ eV/ps}$ the rectification ratio increases to 104%. It indicates that although the increasing of heat flux results in the increasing of rectification ratio, but the rectification ratio is not very sensitive to the heat flux. The result demonstrates that the U-shaped graphene flakes have an obvious advantage in real application. A large rectification effect could be expected even a small amount of heat flux is generated in the nanoelectronic devices.

In order to investigate the influence of the beam upon thermal rectification, different lengths and widths of the beam are studied. The two arms are kept invariant and $J_{\pm} = \pm 0.6 \text{ eV/ps}$ are implemented. In Fig. 4(a) we show that although the rectification effect is enhanced by decreasing the length of the beam, but it is not very sensitive to the length of the beam. Even the length of the beam is much longer than the average length of the two arms ($H_0/((h_L+h_R)/2) = 4.83$), the rectification ratio only decreases to 62%. On the other hand, in Fig. 4(b) we show that the rectification effect is greatly weakened by decreasing the width of beam. When the width of beam

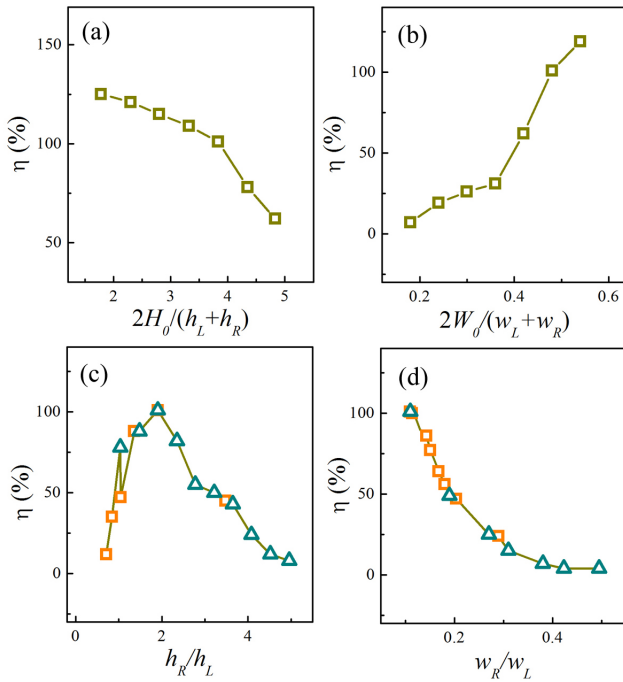


Figure 4: (Color online) (a) Rectification ratio η vs length of the beam. $(h_L + h_R)/2 = 40.9 \text{ \AA}$ and H_0 varies from 72 \AA to 197 \AA . (b) Rectification ratio η vs width of the beam. $(w_L + w_R)/2 = 20.2 \text{ \AA}$ and W_0 varies from 3.6 \AA to 10.9 \AA . (c) Rectification ratio η vs length difference ratio between the two arms h_R/h_L . (d) Rectification ratio η vs width difference ratio between the two arms w_R/w_L . [Triangles in (c) and (d) are obtained by varying the length and width of right arm. Squares in (c) and (d) are obtained by varying the the length and width of left arm.]

is small enough ($W_0/((w_L + w_R)/2) = 0.36$), the rectification ratio decreases to less than 31%.

In order to investigate the effect of structural asymmetry on thermal rectification, different length and width difference ratio of the two arms are studied. In Fig. 4(c) we show that the rectification ratio reaches the maximum value around the length difference ratio $h_R/h_L = 1.91$. It states that although the length asymmetry increases with h_R or h_L , the rectification effect would be weakened by deviating from the proper length difference ratio. Meanwhile, in Fig. 4(d) we show that the rectification ratio increases monotonously with the width difference (since $w_L > w_R$, thus the width difference is greater when w_R/w_L is smaller). It indicates that in real application a large rectification ratio would be expected by introducing a suitable length asymmetry and a large width asymmetry between the two arms.

In summary, we design a thermal rectifier by U-shaped graphene flakes by introducing asymmetric arms. A strong thermal rectification effect is observed and the preferred direction of the heat flux is from the wide arm to the narrow

arm. The rectification ratio is not very sensitive to heatflux which might be important for nanoelectronic devices where only small amount of heat flux is generated. In addition, we state that the proper design of the beam and the structural asymmetry between the two arms are necessary for the rectification effect. Our results may be useful for engineering graphene based nanoelectronic devices.

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